JS 9/13/21
RJA 2/17/22

Ecotox Report for Case # P-18-0238

General

[redacted] [redacted]

Report Status: Complete
Status Date: 09/27/2018
CRSS Date: 07/23/2018
SAT Date: 07/24/2018
SAT Chair: Rebecca Daiss
Consolidated PMN: N
Consolidated Set:
Ecotox Related Cases:
Health Related Cases:
Submitter: Georgia-Pacific Chemicals LLC
CAS Number: None
Chemical Name: [redacted]
Use: [redacted]
Trade Name: None
PV-max(kg/yr): [redacted]
Ecotox Assessor: Jewett, Freeborn

Fate Summary Statement

Fate Summary Statement: P-18-0238
FATE:
EPI estimations for the low weight with 1 of each feedstock, MW = [redacted],
[redacted]
Liquid with MP < 25 °C (E)
log Kow = -0.98 (E)
S
> 10 g/L at 25 °C (E)
VP < 1.0E-6 torr at 25 °C (E)
BP >
400 °C (E)
H < 1.00E-8 (E)
log Koc = 1.00 (E)
log Fish BCF =

0.50 (3) (E)
log Fish BAF = -0.05 (1) (E)
POTW removal (%) = 90-95
via biodeg
Time for complete ultimate aerobic biodeg = wk
Sorption
to soils/sediments = low
PBT Potential: P1B1
*CEB FATE: Migration to
ground water = negl - slow
Bioconcentration factor to be put into
E-FAST: 1

Physical Chemical Information

Molecular Weight: [redacted]

Wt% < 500: **Wt% < 1000:**

Physical State - Neat: Liquid

Melting Point: **Melting Point (est):**

MP (EPI): NaN °C
(Exp.) 349.8399963378906 °C (Est., Joback) 231.32772827148438 °C (Est., Gold) 255.03018188476562 °C (Est., Selected)

Vapor Pressure: **Vapor Pressure (est):** <0.000001

VP (EPI): NaN mmHg (Exp.) 8.59551172933426E-19 Pa
(Est., Antoine) 6.447181807454328E-21 mmHg (Est., Antoine)
2.9480113791488225E-14 Pa (Est., Grain) 2.2111964860629323E-16 mmHg
(Est., Grain) 1.9162998080553697E-10 Pa (Est., Mackay)
1.4373470305391231E-12 mmHg (Est., Mackay) 2.9480113791488225E-14 Pa
(Est., Selected) 2.2111964860629323E-16 mmHg (Est., Selected)
9.501548522202353E-12 Pa (Est., SubCooled) 7.126767166860948E-14 mmHg
(Est., SubCooled)

Water Solubility: **Water Solubility (est):** 1000

Water Solubility (EPI): NaN (Exp.) 4009.865234375
(Est.)

Henry's Law:: NaN atm-m3/mole (Exp.)
2.1760053648975538E-30 atm-m3/mole (Est., Bond)

	2.6209289523585576E-38 atm-m3/mole (Est., Group)		
Log Koc:	NaN	**Log Koc (EPI):**	2.302585092994046 (Est., log(MCI)) -2.813410739111778 (Est., log(Kow)) 10.0 L/kg (Est., MCI) 0.05999999865889549 L/kg (Est., Kow)
Log Kow:		**Log Kow (EPI):**	NaN (Exp.) -0.22 (Est.)
Log Kow Comment:			

SAT Concern Level

Ecotox Rating (1):	1
Ecotox Rating Comment (1):	
Ecotox Rating (2):	
Ecotox Rating Comment (2):	
Ecotox Route of Exposure:	No releases to water

Ecotox Comments

Exposure Based Review (Eco):	Y
Ecotox Comments:	
Exposure Based Testing:	

PBT Ratings

Persistence	Bioaccumulation	Toxicity	Comments
1	1		

Eco-Toxicity Comment:

Fate Ratings

Removal in WWT/POTW (Overall):	90-95					
Condition	**Rating Values**	**Rating Description**				**Comment**
		1	**2**	**3**	**4**	
Fish BCF:	3.16 L/kg wet-wt					
Log Fish BCF:	NaN (Exp.) 0.5 (Est.)					
WWT/POTW Sorption:	1	Low	Moderate	Strong	V. Strong	
WWT/POTW Stripping:	4	Extensive	Moderate	Low	Negligible	
Biodegradation Removal:	2	Unknown	High	Moderate	Negligible	
Biodegradation Destruction:	2-3	Unknown	Complete	Partial	—	
Aerobic Biodeg Ult:	2	<= Days	Weeks	Months	> Months	
Aerobic Biodeg Prim:		<= Days	Weeks	Months	> Months	
Anaerobic Biodeg Ult:	2	<= Days	Weeks	Months	> Months	
Anaerobic Biodeg Prim:		<= Days	Weeks	Months	> Months	
Hydrolysis (t1/2 at pH 7,25C) A:		<= Minutes	Hours	Days	>= Months	
Hydrolysis (t1/2 at pH 7,25C) B:		<= Minutes	Hours	Days	>= Months	
Sorption to Soils/Sediments:	4	V. Strong	Strong	Moderate	Low	
Migration to Ground Water:	1-2	Negligible	Slow	Moderate	Rapid	
Photolysis A, Direct:		Negligible	Slow	Moderate	Rapid	
Photolysis B, Indirect:		Negligible	Slow	Moderate	Rapid	
Atmospheric Ox A, OH:		Negligible	Slow	Moderate	Rapid	
Atmospheric Ox B, O3:		Negligible	Slow	Moderate	Rapid	
Bio Comments:						

Removal in WWT/POTW (Overall):	90-95					
Condition	**Rating Values**	**Rating Description** 1	2	3	4	**Comment**
	[redacted]					Fish log BAF = -0.05 (1). the EPI output file with manually entered properties and the fugacity spreadsheet are attached.
Fate Comments:						

Ecotoxicity Values

Test organism	Test Type	Test Endpoint	Predicted	Experimental	Comments
Fish	96-h	LC50	>100		Predictions (for all structures) are based on the Ecological Structure Activity Relationships [ECOSAR] Predictive Model; specifically the QSAR for esters
Daphnid	48-h	LC50	>100		Predictions (for all structures) are based on the Ecological Structure Activity Relationships [ECOSAR]

Test organism	Test Type	Test Endpoint	Predicted	Experimental	Comments
					Predictive Model; specifically the QSAR for esters
Green Algae	96-h	EC50	>100		Predictions (for all structures) are based on the Ecological Structure Activity Relationships [ECOSAR] Predictive Model; specifically the QSAR for esters
Fish	-	Chronic Value	>10		Predictions (for all structures) are based on the Ecological Structure Activity Relationships [ECOSAR] Predictive Model; specifically the QSAR for esters
Daphnid	-	Chronic Value	>10		Predictions (for all structures) are based on the Ecological Structure Activity Relationships [ECOSAR] Predictive Model;

Test organism	Test Type	Test Endpoint	Predicted	Experimental	Comments
					specifically the QSAR for esters
Green Algae	-	Chronic Value	>10		Predictions (for all structures) are based on the Ecological Structure Activity Relationships [ECOSAR] Predictive Model; specifically the QSAR for esters

Ecotox Value Comments: Predictions (for all structures) are based on the Ecological Structure Activity Relationships [ECOSAR] Predictive Model; specifically the QSAR for esters; MW [redacted]; Log Kow = 0.48 (P, diester), -0.22 (P, diester/monoether), -2.35 (P, triester/monoether); liquid with an unknown MP (P); S = 1E+6 mg/L (P, diester and triester/monoether), 553,000 mg/L (P, diester/monoether); effective concentrations based on 100% active ingredients and mean measured concentrations; hardness <150 mg/L as CaCO3; and TOC <2.0 mg/L.

Ecotox Factors

Factors	Most Sensitive Endpoint	Assessment Factor	CoC	Comment
Acute Aquatic (ppb):	100000	5	20000	The acute COC is based on the fish/aquatic invertebrate L/EC50 toxicity value (Ecological Structure Activity Relationships [ECOSAR] Predictive Model; specifically the QSAR for esters).
Chronic Aquatic(ppb):	10000	10	1000	The chronic COC is based on the fish/aquatic invertebrate chronic value (Ecological Structure Activity Relationships

Factors	Most Sensitive Endpoint	Assessment Factor	CoC	Comment
				[ECOSAR] Predictive Model; specifically the QSAR for esters).

Factors	Values	Comments
SARs:	Esters, Vinyl/Allyl/Propargyl Ethers	
SAR Class:	Esters-vinyl/allyl/propargyl ethers-COOH terminated	
TSCA NCC Category?	Esters	

Recommended Testing: No testing recommendations for ecotoxicity

Ecotox Factors: Environmental Hazard:

Comments: Environmental hazard is relevant to whether a new chemical substance is likely to present unreasonable risk because the significance of the risk is dependent upon both the hazard (or toxicity) of the chemical substance and the extent of exposure to the substance. EPA estimated environmental hazard of this new chemical substance using the Ecological Structure Activity Relationships (ECOSAR) Predictive Model (https://www.epa.gov/tsca-screening-tools/ecological-structure-activity-relationships-ecosar-predictive-model); specifically the QSAR for esters. Acute toxicity values estimated for fish, aquatic invertebrates and algae are all > 100 mg/L. Chronic toxicity values estimated for fish, aquatic invertebrates, and algae are > 10 mg/L. These toxicity values indicate that the new chemical substance is expected to have low environmental hazard. Application of assessment factors of 5 and 10 to acute and chronic toxicity values, respectively, results in acute and chronic concentrations of concern of 20 mg/L (20,000 ppb) and 1 mg/L (1,000 ppb), respectively.

Environmental Risk:
Risks to the environment were evaluated by comparing estimated surface water concentrations with the acute and chronic concentrations of concern. Risks to the environmental were not identified based on low hazard.

Potentially Useful

Information: N/A

Comments/Telephone Log

Artifact	Update/Upload Time
[redacted]	[redacted]